Effective Potential for Ultracold Atoms at the Zero-Crossing of a Feshbach Resonance

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(Dated: September 14, 2010)

We consider finite-range effects when the scattering length goes to zero near a magnetically controlled Feshbach resonance. The traditional effective-range expansion is badly behaved at this point and we therefore introduce an effective potential that reproduces the full T-matrix. To lowest order the effective potential goes as momentum squared times a factor that is well-defined as the scattering length goes to zero. The potential turns out to be proportional to the background scattering length squared times the background effective range for the resonance. We proceed to estimate the applicability and relative importance of this potential for Bose-Einstein condensates and for two-component Fermi gases where the attractive nature of the effective potential can lead to collapse above a critical particle number or induce instability toward pairing and superfluidity. For broad Feshbach resonances the higher-order effect is completely negligible. However, for narrow resonances in tightly confined samples signatures might be experimentally accessible.

PACS numbers: 67.85.-d,03.75.Hh,03.75.Gg,67.85.Lm

INTRODUCTION

Recently there has been extended interesting in weakly interacting Bose-Einstein condensates for use as an atomic interferometer [1] and also to probe magnetic dipolar interactions in condensates [2]. This work was based on ^{39}K atoms where a broad Feshbach resonance exists at a magnetic field strength of $B_0 = 402.4$G [3] which allows a large tunability of the atomic interaction in experiments [4]. Similar tunability has also been reported in a condensate of ^{7}Li [5]. The atomic interaction can be reduced by tuning the scattering length, a, to zero, also known as zero-crossing. In a Gross-Pitaevskii mean-field picture we can thus neglect the usual non-linear term proportional to a. The question is then what other interactions are relevant. As shown in [2], the magnetic dipole will contribute here.

In the Gross-Pitaevskii picture we might also ask whether higher-order terms in the interaction can contribute around zero-crossing. Recently it was shown that effective-range corrections can in fact influence the stability of condensates around zero-crossing [6, 7]. The Feshbach resonances used thus far in experiments have typically been very broad, and as a result the effective range, r_e, will be small, rendering the higher-order terms negligible. However, around narrow resonances this is not necessarily the case and finite-range corrections are not necessarily negligible.

The systematic inclusion of finite-range effects through derivative terms in zero-range models was begun in the study of nuclear matter decades ago [8]. Later on the intricacies of the cut-off problems that arise in this respect was considered by many authors both for the relativistic and non-relativistic case (see [9] for discussion and references). In the context of cold atoms and Feshbach resonances, we need to use a two-channel model [10] in order to take the lowest order finite-range term into

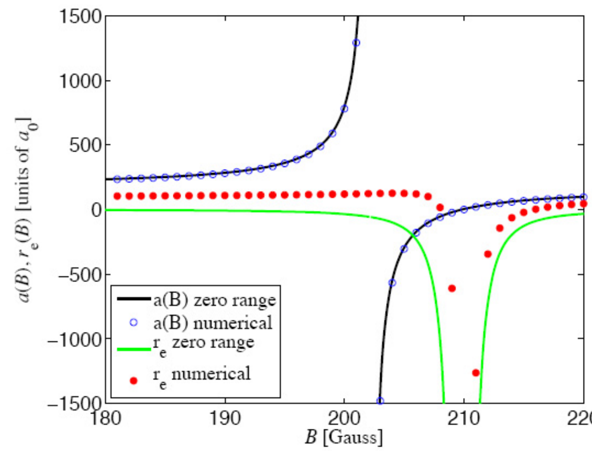

FIG. 1: Scattering length and effective range for the s-wave scattering of fermionic ^{40}K atoms around the Feshbach resonance at $B_0 = 202.1$ G demonstrating the divergence in a coupled-channel calculation (symbols) [13] and in a zero-range model (full lines). The difference in the zero-range and coupled-channel models is caused by the presence of a bound state close to threshold in the open channel.

account. Similar models were already introduced in [11] and denoted resonance models (see f.x. [12] for a comprehensive review of scattering models for ultracold atoms). We note that whereas resonance models treat the closed-channel molecular state as a point boson the model of [10] treats the molecule more naturally as a composite object of two atoms. In the end the parameters of the two models turn out to be similarly related to the physical parameters of Feshbach resonances. In Fig. (1) we show calculations of scattering length and effective range for the Feshbach resonance at $B = 202.1$ G in ^{40}K in both a coupled-channel model [13] and in the zero-range model discussed here. We see the effective range being roughly constant at resonance and then start to diverge

at zero-crossing. The zero-range model provides a good approximation to the full calculations and for many-body purposes it is preferable due to its simplicity. Whereas the earlier work of [11] considered the regime close to the resonance, we will be exclusively concerned with zero-crossing. To our knowledge the intricacies of this region have not been addressed in the literature in the context of Feshbach resonances.

Around zero-crossing the Feshbach model turns out to have a badly behaved effective-range expansion. The parameters obtained from the effective-range expansion should therefore be used with extreme caution as the series is divergent at this point. However, as we show in this article, the finite-range corrections obtained from the full T-matrix at low momenta via an effective potential turn out to be the same as one would naively expect based on the effective-range expansion. After introducing the effective potential we consider its applicability and importance in the case of Bose-Einstein condensates and for two-component Fermi gases where the attractive nature of the effective interaction at zero-crossing could lead to collapse above a certain critical particle number or to pairing instability and superfluidity. In general, we find that tight external confinement is a necessary condition for the higher-order effects to dominate the magnetic dipole interaction and be experimentally observable.

TWO-CHANNEL MODEL

We consider a two-channel s-wave Feshbach model with zero-range interactions [10] for which the on-shell open-open channel T-matrix as a function of magnetic field, B, is

$$T_{oo}(B) = \frac{\frac{4\pi\hbar^2}{m} a_{bg}}{\left(1 + \frac{\Delta\mu\Delta B}{\frac{\hbar^2 q^2}{m} - \Delta\mu(B - B_0)}\right)^{-1} + i a_{bg} q}, \quad (1)$$

where $\Delta\mu$ is the difference between the magnetic moments in the open and closed channel, q is the relative momentum of the atoms of mass m, a_{bg} is the scattering length away from the resonance at magnetic field B_0, and ΔB is the width of the resonance. We can compare this to the standard vacuum expression for the T-matrix in terms of the phase-shift given by

$$T_v(B) = \frac{\frac{4\pi\hbar^2}{m} a}{-qa \cot\delta(q) + iaq}, \quad (2)$$

where $a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right)$ as in the commonly employed single-channel models. From Eqs. (1) and (2) we obtain the relation for the phase-shift

$$q \cot\delta(q) = \frac{-1}{a_{bg}} \left(1 + \frac{\Delta\mu\Delta B}{\frac{\hbar^2 q^2}{m} - \Delta\mu(B - B_0)}\right)^{-1}. \quad (3)$$

We now expand the right-hand side in powers of q as is usually done in an effective-range expansion. This yields

$$q \cot\delta(q) = \frac{-1}{a(B)} + \sum_{n=1}^{\infty} \frac{-1}{a_{bg}} \left[\frac{-a_{bg} r_{e0}}{2}\right]^n \left[\frac{a_{bg}}{a(B)} - 1\right]^{n+1} q^{2n}, \quad (4)$$

where $r_{e0} = -2\hbar^2/(m\Delta B\Delta\mu a_{bg})$ is the background value of the effective range around the resonance. From Eq. (4) we can now read off all coefficients in an effective-range expansion with their full B-field dependence. For instance, the effective range is given simply by $r_e = r_{e0}\left[\frac{a_{bg}}{a} - 1\right]^2$, which is divergent when $a(B) \to 0$. We also clearly see that all the other coefficients are divergent in that limit. This is signaled also before doing the full expansion in q as the first term in Eq. (4) diverges at zero-crossing. However, in effective potentials derived from the T-matrix these problems are not transparent as the lowest order coefficient is proportional to $a(B)$ (see Eq. (11)). Below we will discuss what kind of constraints this introduces on the applicability of the effective-range expansion near zero-crossing. We note that similar issues were briefly discussed in a different context in [14] where an equivalent to Eq. (6) below was obtained.

Let us first consider the low-q limit and compare the full T-matrix with the effective-range expansion as zero-crossing is approached. Taking the low-q limit of Eq. (3) at zero-crossing where $\Delta B/(B - B_0) = 1$, we find

$$q \cot\delta(q) \to \frac{-1}{a_{bg}} - \frac{\Delta\mu\Delta B}{\frac{\hbar^2 q^2}{m}}, \quad (5)$$

which diverges as q^{-2}. Therefore the coefficients of the expansion in Eq. (4) must necessarily diverge in order to retain any hope of describing the low-q behavior. Furthermore, since the expansion is an alternating series and therefore slowly converged, we also conclude that many terms must be retained for a fair approximation at very small but non-zero q. The same conclusion can be reached by considering the radius of convergence of Eq. (4), which we find by locating the pole in Eq. (3) at $\hbar^2 q^2/m = \Delta\mu(B - B_0 - \Delta B)$. This radius indeed goes to zero at zero-crossing. We are thus forced to conclude that the effective-range expansion breaks down near zero-crossing.

Effective Potential at Zero-crossing

Since the effective-range expansion is insufficient we consider the full T-matrix in the low-q limit at zero-crossing. To lowest order we have

$$T_{oo}(B = B_0 + \Delta B) = -\frac{4\pi\hbar^2 a_{bg}}{m} \frac{\hbar^2 q^2}{m\Delta\mu\Delta B} + O(q^4). \quad (6)$$

Using the expression for r_{e0}, this can be written

$$\frac{4\pi\hbar^2}{m}\frac{a_{bg}^2 r_{e0}}{2}q^2. \tag{7}$$

Knowing the T-matrix at low q we can now proceed to find an effective low-q potential through the Lippmann-Schwinger equation

$$V = T - TG_0V, \tag{8}$$

where $G_0 = (E - H_0 + i\delta)^{-1}$ is the free space Green's function [15]. This equation can be solved for $T(q,q') \propto q^2 + {q'}^2$ (the symmetrized version of the full T-matrix) in an explicit cut-off approach [9, 15] and then be expanded to order q^2 for consistence with the input T-matrix. In the long-wavelength limit we can take the cut-off to zero [15] and for the on-shell effective potential we then obtain the obvious answer

$$V(q) = \frac{4\pi\hbar^2}{m}\frac{a_{bg}^2 r_{e0}}{2}q^2 \tag{9}$$

in momentum space. The effective potential in real-space is now easily found by canonical substitution ($\boldsymbol{q} \to -i\nabla$) and appropriate symmetrization [16]. We have

$$V(\boldsymbol{r}) = -\frac{4\pi\hbar^2}{m}\frac{a_{bg}^2 r_{e0}}{2}\frac{1}{2}\left[\overleftarrow{\nabla}_{\boldsymbol{r}}^2\delta(\boldsymbol{r}) + \delta(\boldsymbol{r})\overrightarrow{\nabla}_{\boldsymbol{r}}^2\right]. \tag{10}$$

Notice that the Lippmann-Schwinger approach is non-perturbative as opposed to the perturbative energy shift method [16, 17].

Comparison to Effective-Range Expansion and Energy-Shift Method

Away from zero-crossing one can easily relate the effective-range expansion to an effective potential through the perturbative energy shift method [9, 16, 17]. To second order the s-wave effective potential is

$$V(\boldsymbol{r}) = \frac{4\pi\hbar^2 a}{m}\left[\delta(\boldsymbol{r}) + \frac{g_2}{2}\left(\overleftarrow{\nabla}_{\boldsymbol{r}}^2\delta(\boldsymbol{r}) + \delta(\boldsymbol{r})\overrightarrow{\nabla}_{\boldsymbol{r}}^2\right)\right], \tag{11}$$

where the first term is the effective interaction usually employed in mean-field theories of cold atoms [15]. In terms of a and r_e, we have $g_2 = a^2/3 - ar_e/2$ [16, 17] with the field-dependent $a = a(B)$ and $r_e = r_e(B)$.

At zero-crossing the first term in Eq. (11) vanishes and one might expect the second term to vanish as well. However, in the naive effective-range expansion of the two-channel model discussed above we saw that r_e diverges as a^{-2} and we therefore have

$$\lim_{a\to 0} ag_2 = -\frac{a_{bg}^2 r_{e0}}{2}. \tag{12}$$

In particular, if we for a moment ignore q^4 terms in the effective-range expansion, we recover exactly the same effective potential as in Eq. (10) at zero-crossing. The finite limiting result in Eq. (12) shows that the potential in Eq. (11) is well-defined as $a \to 0$, provided that appropriate regularization and renormalization is performed. Eq. (11) thus applies equally well at resonance ($a \to \infty$) where the gradient terms are small and at zero-crossing where the lowest order delta function term is unimportant. It is thus a well-defined effective potential over the entire range of a Feshbach resonance.

We therefore see that even though the effective-range expansion has divergent coefficients at zero-crossing, the lowest order does in fact give the same effective potential as the full T-matrix if we apply it naively. The effective-range expansion should thus be viewed as an asymptotic series. However, we cannot use the effective-range expansion to estimate the validity of the second order effective potential since the radius of convergence goes to zero at zero-crossing as discussed above.

RELATION TO EXPERIMENTS

Above we only retained terms of order q^2 in the full T-matrix. We now estimate the energy regime in which this expression is valid. Demanding that the q^4 term be smaller than the q^2 term gives the criterion

$$\frac{\hbar^2 q^2}{m} \ll \frac{\hbar^2}{m|a_{bg}r_{e0}|}. \tag{13}$$

We relate this condition to recent experiments with bosonic condensates of ^{39}K working around zero-crossing [1]. The resonance used there is very broad ($\Delta B = -52$G) with $a_{bg} = -29a_0$ and $r_{e0} = -58a_0$ (a_0 is the Bohr radius). The right-hand side of Eq. (13) is $2.3\cdot 10^{-7}$ eV, corresponding to a temperature of about 3 mK. Since the experiments are performed at much lower temperatures the approximation above is certainly valid. However, as a_{bg} and particularly r_{e0} is small, the front factor in Eq. (10) is also small. The relevant scale of comparison is the outer trap parameter b [6] which is typically of order 1μm, yielding a vanishing ratio $|a_{bg}^2 r_{e0}|/b^3 \sim 10^{-9}$. For broad Feshbach resonances the higher-order interactions can thus be safely ignored. For very narrow resonances the situation potentially changes as r_{e0} can be very large and make the potential in Eq. (10) important. As an example, we consider the narrow resonance in ^{39}K at $B_0 = 25.85$G with $\Delta B = 0.47$G, $a_{bg} = -33a_0$, and $r_{e0} = -5687a_0$ [3]. The right-hand side of Eq. (13) is now $2\cdot 10^{-9}$ eV, corresponding to 24 μK. This is again much higher than experimental temperatures. A more careful argument can be made from the energy per particle of the non-condensed cloud. Ignoring the trap, we have $E/N = 0.770 k_B T_c (T/T_c)^{5/2}$ (T_c is the critical temperature) [15]. For a sample of $3\cdot 10^4$ a critical temperature of 100 nK was reported in [4]. Using this T_c we find that $T \ll 900$nK for Eq. (13) to hold. Again this is within the

experimental regime. The effective potential approach should therefore be applicable around zero-crossing for narrow resonances. However, even with this narrow resonance we find $|a_{bg}^2 r_{e0}|/b^3 \sim 10^{-7}$ and the effect is still completely negligible.

In order to increase the relevance of the higher-order term, we now consider some very narrow resonances that have been found in ^{87}Rb. In particular, the resonance at $B_0 = 9.13$G [18] which was recently utilized in nonlinear atom interferometry [19]. We have $\Delta B = 0.015$G, $a_{bg} = 99.8a_0$, and $\Delta\mu = 2.00\mu_B$ [20], which gives $r_{e0} = -19.8 \cdot 10^3 a_0$ and a ratio $|a_{bg}^2 r_{e0}|/b^3 = 2.92 \cdot 10^{-5}(1\mu\text{m}/b)^3$. A trap length of $b \sim 0.5\mu$m as used in [19] would thus yield 10^{-4} and demonstrates that higher-order corrections can safely be neglected. For a ratio of 1 we need $b \sim 0.03\mu$m which is unrealistically small in current traps or optical lattices. However, a resonance of width $\Delta B = 0.0004$G is known in the same system at $B_0 = 406.2$G [21] with $a_{bg} = 100a_0$ and $\Delta\mu = 2.01\mu_B$ [20]. In this case we find $r_{e0} = -7.4 \cdot 10^5 a_0$ and a much more favorable ratio of $|a_{bg}^2 r_{e0}|/b^3 = 0.001(1\mu\text{m}/b)^3$. Here we see that a ratio of 1 is achieved already for $b \sim 0.1\mu$m which not far off from tight traps or optical lattice dimensions. In terms of temperature we still have to be in the ultralow regime of $T \lesssim 30$nK according to Eq. (13) for the latter resonance.

Consider now a fermionic two-component system where s-wave interactions are dominant. Since we have $r_{e0} < 0$ for all Feshbach resonances [20], the effective potential in Eq. (9) is attractive and the system could potentially be unstable toward a paired state or become unstable to collapse above a critical particle number. For simplicity we will use the semi-classical Thomas-Fermi approach to describe a gas with equal population of the two components and estimate the critical particle number. Assuming an isotropic trapping potential with length scale $b = \sqrt{\hbar/m\omega}$ where ω is the trap frequency, the ground-state density, $\rho(\boldsymbol{x})$, can be found by minimization and satisfies

$$\left[\frac{\mu}{\hbar\omega} - \frac{1}{2}\left(\frac{\boldsymbol{x}}{b}\right)^2\right] = \frac{1}{2}(k_F(\boldsymbol{x})b)^2 - \frac{4}{30\pi}\alpha(k_F(\boldsymbol{x})b)^5, \quad (14)$$

where $\rho(\boldsymbol{x}) = k_F(\boldsymbol{x})/6\pi^2$ and $\alpha = a_{bg}^2|r_{e0}|/b^3$. The maximum allowed momentum and chemical potential, μ, is found by solving for the turning point of the right-hand side of Eq. (14) which gives

$$k_{max}b = \left[\frac{3\pi}{2\alpha}\right]^{1/3} \quad \text{and} \quad \mu_{max} = \frac{3}{10}\hbar\omega(k_{max}b)^2. \quad (15)$$

We can now compare this k_{max} to the value obtained from the non-interacting density within the Thomas-Fermi approximation at the center of the trap. In terms of the number of particles in each component, N, at the center of the trap we have $k_F(0)b \approx 1.906N^{1/6}$ [15]. By equating these two expression we obtain an estimate for the critical number of particles, N_{max}. Inserting the relevant units, we have

$$N_{max} = 2 \cdot 10^{25}\left(\frac{a_0}{a_{bg}}\right)^4\left(\frac{a_0}{r_{e0}}\right)^2\left(\frac{b}{1\,\mu\text{m}}\right)^6, \quad (16)$$

where a_0 is the Bohr radius. We note that the scaling $N_{max} \propto \alpha^{-2}$ can also be obtained by considering the point at which the monopole mode becomes unstable.

Typical numbers for common fermionic species ^{6}Li or ^{40}K in the lowest hyperfine states [20] lead to $N_{max} \sim 10^{12}$ for $b = 1\,\mu$m. This is of course a huge number and experiments are well within this limit. Even if one reduced the trap length by a factor of ten and made the presumably unrealistic assumption that the particle number remains the same we still have $N \ll N_{max}$. The reason is that the s-wave Feshbach resonances utilized in the two-component gases are generally broad in order to study the universal regime. If we consider the narrow resonance at $B_0 = 543.25$G in ^{6}Li [22] with $\Delta B = 0.1$G, $a_{bg} = 60a_0$, and $\Delta\mu = 2.00\mu_B$ [20], we have $N_{max} \sim 2 \cdot 10^{13}(b/1\mu\text{m})^6$. This is somewhat better but we still need $b \sim 0.06\mu$m to get to an experimentally relevant $N_{max} \sim 10^6$. We have to conclude that higher-order s-wave interactions are highly unlikely to be observable through monopole instabilities. In light of this it seems better to consider p-wave resonances which are much more narrow in general. However, also here extremely small trap sizes appear necessary [23].

The instability toward Cooper pairing around zero-crossing can also be estimated in simple terms. In general the critical temperature is $T_c \sim T_F \exp(-1/N_0|U|)$, where $N_0 = mk_F(0)/2\pi^2\hbar^2$ is the density of states at the Fermi energy in the trap center and $U < 0$ is a measure of the attraction. For the latter we use the effective potential in momentum space from Eq. (9) and make the assumption that $q \sim k_F(0)$. Using the expression for $k_F(0)$ in terms of N above, we find

$$\frac{1}{N_0|U|} = \frac{1.5 \cdot 10^{12}}{\sqrt{N}}\left(\frac{b}{1\,\mu\text{m}}\right)^3\left(\frac{a_0}{a_{bg}}\right)^2\frac{a_0}{|r_{e0}|}. \quad (17)$$

For broad resonances in ^{6}Li or ^{40}K this exponent is of order 10^3 and T_c is thus vanishingly small. However, the scaling with trap size can help and if we imagine reducing to $b = 0.1\,\mu$m, we find $T_c \lesssim 0.5T_F$ for $N = 10^6$ atoms. For the narrow resonance in ^{6}Li discussed above, we find that $T_c \sim 0.5T_F$ with $N = 10^6$ can be achieved for $b \sim 0.5\mu$m and $T_c \sim 0.1T_F$ for $N = 10^5$. Thus there may be a possibility to reach the pairing instability near zero-crossing if high particle numbers can be cooled in tight traps and narrow resonances are used.

Dipole-Dipole Interactions

The discussion above ignores the dipole-dipole interaction discussed in the introduction which will compete

against the higher-order effective potential from the Feshbach resonance. A simple estimate can be made along the lines of the discussion in [15]. The external trapping potential is the characteristic scale of spatial variations and we thus find a ratio, r, of magnetic dipole-dipole, U_{md}, to higher-order s-wave zero-range interaction strength, U_2, which can be written as

$$r = \frac{U_{md}}{U_2} = \frac{a_0 b^2}{a_{bg}^2 |r_{e0}|} = 35.7 \left[\frac{b}{1\mu\text{m}}\right]^2 \left[\frac{100a_0}{a_{bg}}\right]^2 \frac{1000a_0}{|r_{e0}|}. \tag{18}$$

For $r < 1$ the higher-order interaction term will therefore dominate the magnetic dipole term. For the case of narrow resonances in ^{87}Rb discussed above we find $r \sim 0.11(b/1\mu\text{m})^2$ for the resonance at $B_0 = 9.13$G and $r \sim 0.05(b/1\mu\text{m})^2$ for the one at $B_0 = 406.2$G. For the narrow resonance in ^{6}Li at $B_0 = 543.25$G we find $r \sim 1.4(b/1\mu\text{m})^2$. These ratios clearly indicate that magnetic dipole-dipole interactions can be suppressed relative to higher-order zero-range terms for narrow Feshbach resonances and standard trap sizes. This dominanace becomes even stronger for the tight traps needed for the realization of the effects discussed above and we thus conclude that interference of the magnetic dipole-dipole term is not a major concern.

CONCLUSIONS

In this article we have discussed the effective potential around a Feshbach resonances as the scattering length is tuned to zero and finite-range corrections become important. We showed that the effective-range expansion is badly behaved and the effective potential most be defined from the T-matrix. We have demonstrated that the low momenta effective potential obtained from the full T-matrix agrees with one obtained naively from the effective-range expansion when the scattering length goes to zero. Thus even though the effective-range expansion has divergent coefficients at zero-crossing the first terms of the associated effective potential yield consistent results. We then estimated the effects of the terms on different condensates. Since the effective potential at zero-crossing is attractive it may induce various instabilities which we considered for the case of a two-component Fermi gas under harmonic confinement.

For the broad Feshbach resonances used in current experiments the effective potential discussed here are negligible and the dipole-dipole interaction dominates completely at zero-crossing. However, for narrow resonances in very tightly confined systems some of the effects might be detectable. The competing dipole interaction is small for narrow resonances in tight confinement. However, it is conceivable that effects of spherically symmetric higher-order terms could be separated from dipolar effects which change with system geometry [2].

Acknowledgments The author would like to thank Martin Thøgersen for very fruitful collaborations. Correspondence with Georg Bruun about two-channel models is highly appreciated. We are grateful to Nicolai Nygaard for discussions and for producing Fig. (1). This work was supported by the Villum Kann Rasmussen foundation.

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